Numerical Simulation of Plastic-Bonded Explosives

Scott Bardenhagen and Andrew Brydon (T-14)

Homogeneous continuum models have been developed to describe the response of material to dynamic loading, including equation of state, strength, and reactive burn models. However many strategic materials—in particular plastic-bonded explosives (PBXs)—are heterogeneous at the microscale. PBXs are composites containing energetic grains, ranging in size from less than one to a few hundred micrometers, embedded in a matrix of high-polymer binder. Low levels of applied stress can cause substantial material damage and even lead to violent reactions due to the heterogeneity of the material state at the microscale.

To develop accurate, quantitative, and predictive models, it is imperative to develop a sound physical understanding of the grain-scale material response. The orientationally dependent properties of the individual crystals and the presence of material interfaces result in strongly heterogeneous stress and energy distribution under loading. Because events of interest such as damage and chemical decomposition depend strongly on the extremes (tails) of these distributions, it is important to understand what factors affect them. The goal of this work is to characterize the heterogeneity of stress and energy distribution as a function of material microstructure.

The Material Point Method (MPM) has been used to perform numerical simulations indicating the importance of accurately modeling microscale composite material response. The computational technique is a particle method that provides a convenient framework for tracking and modeling material interfaces. Stress wave propagation simulations on idealized composite microstructures, granular packings consisting of photoelastic polymeric cylinders, illustrate differences in stress distributions due to granular contact conditions (see Fig. 1).

More recently, advantages of the MPM for discretizing geometrically complex material microstructures have been exploited. In particular, the compatibility of particle discretization and x-ray microtomography has been demonstrated [1]. X-ray microtomography generates three-dimensional (3-D) spatial variation of a composite's x-ray cross section (see Fig. 2). For PBXs, a sophisticated image-processing step is required to extract individual entities (individual grains, binder). Once constituents have been identified, discretization via particles is straightforward.

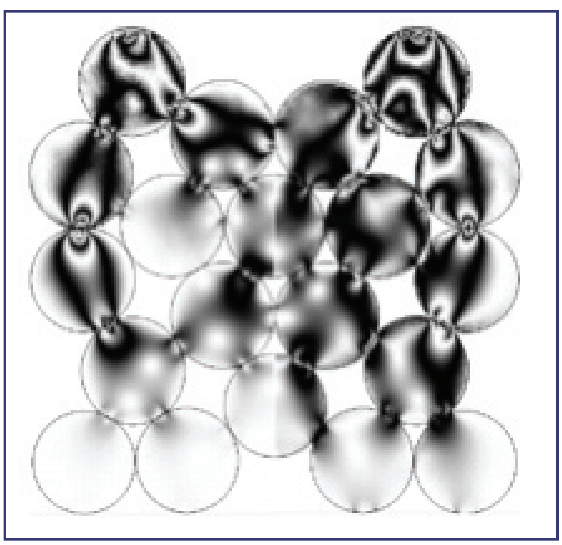

***Figure 1—* Wave propagation through a collection of disks. Frictionless contact (left) is contrasted with no slip contact (right).**

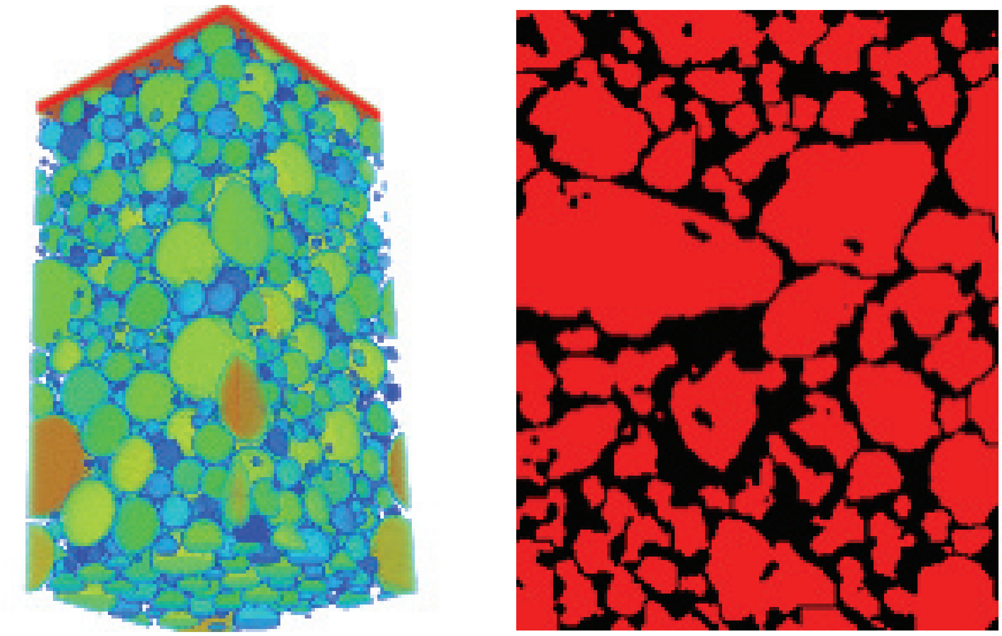

Figure 2—
Idealized (left) 3D granular packing and experimentally obtained (right) 2D slice through a PBX.

Researchers S. Lecume and C. Boutry, SNPE, Centre de Recherches du Bouchet, France, have obtained 3D x-ray microtomography data for a particular formulation (PBX N109), analyzed this data, and successfully extracted individual grains and binder. We are collaborating with SNPE to replace existing idealized models (packed spheres) with experimentally obtained granular packings. We have received one data set and are in the process of discretizing it in order to assess the impact of grain shape on material state distribution under various loadings.

[1] Andrew Brydon and Scott Bardenhagen, "Numerical Simulation of Realistic Foam Microstructures," in this volume on p. 36.

For more information, contact Scott Bardenhagen (bard@lanl.gov).

Acknowledgements
We would like to acknowledge NNSA's Advanced Simulation and Computing (ASC), Materials and Physics Program; and Campaign 2, Dynamic Materials Properties, for financial support.